# Bell inequalities for maximally entangled states 

Alexia Salavrakos ${ }^{1}$, Remigiusz Augusiak ${ }^{2}$, Jordi Tura ${ }^{1}$, Peter Wittek ${ }^{1,3}$, Antonio Acín ${ }^{1,4}$, Stefano Pironio ${ }^{5}$<br>${ }^{1}$ ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Barcelona, Spain<br>${ }^{2}$ Center for Theoretical Physics, Polish Academy of Sciences, Aleja Lotników 32/46, 02-668 Warsaw, Poland<br>${ }^{3}$ University of Borås, Allegatan 1, 50190 Borås, Sweden<br>${ }^{4}$ ICREA, Pg. Lluis Companys 23, 08010 Barcelona, Spain<br>${ }^{5}$ Laboratoire d'Information Quantique, CP 224, Université libre de Bruxelles (ULB), 1050 Bruxelles, Belgium


#### Abstract

Bell inequalities have traditionally been used to demonstrate that quantum theory is nonlocal, in the sense that there exist correlations generated from composite quantum states that cannot be explained by means of local hidden variables. With the advent of deviceindependent quantum information processing, Bell inequalities have gained an additional role as certificates of relevant quantum properties. In this work we consider the problem of designing Bell inequalities that are tailored to detect the presence of maximally entangled states. We introduce a class of Bell inequalities valid for an arbitrary number of measurements and results, derive analytically their maximal violation and prove that it is attained by maximally entangled states. Our inequalities can therefore find an application in deviceindependent protocols requiring maximally entangled states.


## 1 Introduction

Measurements on separated subsystems in a joint entangled state may display correlations that cannot be mimicked by local hidden variable models. These correlations are known as nonlocal, and they are detected by violating the so-called Bell inequalities $[1,2]$. In recent years, however, it has been become clear that non-locality is interesting not only for fundamental reasons, but also as a resource for many device-independent (DI) quantum information tasks [2], such as quantum key distribution [3, 4] or random number generation [5, 6]. From this new point of view, the violations of Bell inequalities are not merely indicators of non-locality, but can be used to infer qualitative and quantitative statements about different operationally relevant quantum properties.

Traditionally, the construction of Bell inequalities has been addressed from the point of view of deriving constraints satisfied by local models. Following this standard approach, the inequalities are constructed using well-known techniques in convex geometry. Indeed, the set of correlations admitting a local hidden variable model corresponds to a polytope [2], that is, a convex set with a finite number of extreme points or vertices. These vertices are known and correspond to local deterministic assignments, while the (in general) unknown facets are the desired Bell inequalities. Such "facet Bell inequalities" form a complete set of Bell inequalities, in the sense that they provide necessary and sufficient criteria to detect the non-locality of
given correlations. Clauser-Horne-Shimony-Holt (CHSH) [7] and Collins-Gisin-Linden-MassarPopescu (CGLMP) [8] inequalities are examples of tight inequalities.

If such facet Bell inequalities are optimal detectors of non-locality, they are, however, not necessarily optimal for inferring specific quantum properties in the device-independent setting. For instance, in a scenario where two binary measurements are performed on two entangled subsystems, it is well known that the violation of the CHSH inequality [7] is a necessary and sufficient condition for non-locality. But certain "non-facet" Bell inequalities are better certificates of quantum randomness than the CHSH inequality when the two quantum systems are partially entangled [9].

In the present work, we consider the problem of constructing Bell inequalities whose maximal quantum violation, usually referred to as the Tsirelson bound [10], is attained for maximally entangled states of two qudits. This is a desirable property since such states have particular features, such as perfect correlations between outcomes of local measurements in the same bases, and therefore many quantum information protocols rely on them. The main aim of this work is to introduce a family of Bell inequalities with an arbitrary number of measurements and outcomes which are maximally violated by the maximally entangled pair of two qudits. Crucially, their maximal quantum violation can be computed analytically.

In the case where only two measurements are made on each subsystem, all facet Bell inequalities are known for a small number of outputs and they are all of the CGLMP form [8]. However, the CGLMP inequalities are not maximally violated by the maximally entangled states of two qudits (except in the case $d=2$ corresponding to the CHSH inequality) [ $11,12,13]$. We should therefore not expect a priori our inequalities to be facet inequalities, and indeed they are not.

The fact that our inequalities will not necessarily be facet inequalities also implies that we cannot use standard tools based on convex geometry and polytopes to construct them. In fact, no quantum property is used for the construction of tight Bell inequalities like CGLMP and, in this sense, it may not be that surprising that their maximal violation does not require maximal entanglement. Our approach is completely different: it starts instead from quantum theory and exploits the symmetries and perfect correlations of maximally entangled states to derive a Bell inequality. It is also closely linked to sum of squares decompositions of the Bell operator, which can be used to determine their Tsirelson bound. Thus, quantum theory becomes a key ingredient of our method for generating new Bell inequalities.

Our results have the potential to be used in DI quantum information protocols. The inequalities are good candidates for improved DI random number generation or quantum key distribution protocols or to self-test [14] maximally entangled states of high dimension. Interestingly, they also give further insight into the structure of the set of quantum correlations.

The paper is organized as follows: in Section 2, we review the necessary framework to state our results. In Section 3 we introduce our Bell inequalities and their derivation, while in Section 4 we study their properties and give their Tsirelson bound. In Sections 5 and 6, we briefly discuss their possible application to DI protocols and the interest of our findings.

## 2 Preliminaries

Throughout this work, we consider a bipartite Bell scenario in which two distant parties $A$ and $B$ (often taking the placeholder names Alice and $B o b$ ) perform measurements on their share of some physical system. We suppose that they have $m$ possible measurement choices (or inputs) at their disposal and that each measurement has $d$ possible outcomes (or outputs). We denote this scenario $(2, m, d)$. We label their inputs and outputs as $x, y \in\{1, \ldots, m\}$ and $a, b \in\{0, \ldots, d-1\}$. The correlations that can be obtained in such a Bell experiment are described by a set of $(m d)^{2}$ joint probabilities $P\left(A_{x}=a, B_{y}=b\right)$ that Alice and Bob obtain $a$
and $b$ upon performing the $x$ th and $y$ th measurement, respectively. These probabilities can be given a geometric representation by ordering them into a vector

$$
\begin{equation*}
\vec{p}:=\left\{P\left(A_{x}=a, B_{y}=b\right)\right\}_{a, b, x, y} \in \mathbb{R}^{(m d)^{2}} \tag{1}
\end{equation*}
$$

Importantly, the set of allowed $\vec{p}$ can vary, depending on the physical principles the probabilities $P\left(A_{x}=a, B_{y}=b\right)$ obey. Thus, to every physical theory, one can assign a set of correlations in $\mathbb{R}^{(m d)^{2}}$. If the measurements correspond to spacelike separated events, the observed correlations should obey the no-signalling principle, which prevents any faster-than-light communication among the parties. These correlations form a convex set that is a polytope, which we denote by $\mathcal{N}$. Contained in this set is the set of quantum correlations, denoted $\mathcal{Q}$, which corresponds to those $\vec{p}$ whose components can be written as

$$
\begin{equation*}
P\left(A_{x}=a, B_{y}=b\right)=\langle\psi| P_{a}^{(x)} \otimes P_{b}^{(y)}|\psi\rangle \tag{2}
\end{equation*}
$$

where $|\psi\rangle$ is some state in a tensor product Hilbert space $H_{A} \otimes H_{B}$ whose dimension is unconstrained, and $\left\{P_{a}^{(x)}\right\}$ and $\left\{P_{b}^{(y)}\right\}$ are projection operators defining, respectively, the measurement $x$ on Alice's system and the measurement $y$ on Bob's system. Finally, the set of correlations admitting local hidden variable models, termed also local or classical, corresponds to those $\vec{p}$ that can be written as a convex sum of product deterministic correlations of the form $P\left(A_{x}=a, B_{y}=b\right)=\delta_{a, \kappa_{x}} \delta_{b, \lambda_{y}}$ where $\kappa_{x}$ and $\lambda_{y}$ denote Alice's and Bob's predetermined outputs for inputs $x$ and $y$, respectively.

Bell was the first to prove that not all quantum correlations admit a local hidden variable model [1]. To this end, he used the concept of a Bell inequality $I \leq C_{b}$ with $I$ being the so-called Bell expression that, most generally, is a linear combination of the $(m d)^{2}$ joint probabilities of the form

$$
\begin{equation*}
I:=\sum_{a b x y} I_{a b x y} P\left(A_{x}=a, B_{y}=b\right) \tag{3}
\end{equation*}
$$

and $C_{b}$ is the local (or classical) bound of the Bell inequality and it is the maximum value

$$
\begin{equation*}
C_{b}=\max _{\kappa_{x}, \lambda_{y}} \sum_{a b x y} I_{a b x y} \delta_{a, \kappa_{x}} \delta_{b, \lambda_{y}} \tag{4}
\end{equation*}
$$

that $I$ can achieve on product deterministic correlations [15]. The quantum or Tsirelson bound of the Bell expression is the maximum value

$$
\begin{equation*}
Q_{b}=\sup _{|\psi\rangle,\left\{P_{a}^{(x)}\right\},\left\{P_{b}^{(y)}\right\}} \sum_{a b x y} I_{a b x y}\langle\psi| P_{a}^{(x)} \otimes P_{b}^{(y)}|\psi\rangle \tag{5}
\end{equation*}
$$

that it can achieve for quantum correlations. Such a Bell expression corresponds to a proper Bell inequality - one that can be violated by quantum theory - if $C_{b}<Q_{b}$. Let us finally define $N S_{b}$ to be the maximal value of $I$ over all no-signalling correlations. It turns out that for most Bell inequalities the chain of inequalities $N S_{b}>Q_{b}>C_{b}$ holds true [1, 16, 17].

The set of local correlations is a polytope which is defined through Bell inequalities. Hence, if $\vec{p}$ violates a Bell inequality, the correlations described by $\vec{p}$ are nonlocal. The set $\mathcal{Q}$, on the other hand, is not a polytope, yet it is convex. There have been several attempts to characterize it from an operational point of view $[18,19,20]$, but an operational characterization remains to be found [21]. The main obstacle is the current lack of mathematical understanding of the structure of the set of quantum correlations. This makes the derivation of Tsirelson bounds a difficult problem. Indeed, given an arbitrary Bell inequality, there is no procedure that guarantees finding its Tsirelson bound, and it was achieved analytically only in a handful of cases. There is however a
practical approximation scheme introduced in [13] based on a semidefinite programming, which consists in a hierarchy of sets $\mathcal{Q}_{1} \supseteq \mathcal{Q}_{2} \supseteq \cdots \supseteq \mathcal{Q}_{k} \supseteq \ldots$ converging to $\mathcal{Q}$ as $k \rightarrow \infty$. The sets $\mathcal{Q}_{k}$ are the feasible regions of semi-definite programs, which are efficiently solvable. Although this method yields in practice very good upper numerical bounds (often tight ones) on the maximal violations of Bell inequalities for small Bell scenarios, it is limited by the fact that it becomes computationally expensive for larger scenarios and for high $k$.

## 3 Class of Bell expressions

As stated in the introduction, our aim is to introduce a family of Bell expressions, whose maximal quantum value is attained by the maximally entangled states of two qudits $\left|\psi^{+}\right\rangle=$ $(1 / \sqrt{d}) \sum_{i=0}^{d-1}|i i\rangle$. To derive these Bell expressions, we start from the premise that their maximal quantum values are obtained when Alice and Bob perform the optimal CGLMP measurements introduced in $[22,8]$ for the case $m=2$ and generalized to more inputs in [23]. The reason for this choice is that these measurements simply generalize the CHSH measurements $(d=2)$ to the case $d>2$ and that they lead to non-local correlations that are the most robust to noise [22] or give a stronger statistical test [24] (at least in the case $m=2$ ). These measurements are presented in detail in Appendix A.

Note that this choice of measurements is arbitrary and only used as a starting point to determine the Bell expressions that we are looking for. But once we have determined them, we will no longer make any assumptions on the particular measurements that Alice and Bob perform, in particular, when we derive formally their quantum bounds.

The probabilities $P\left(A_{x}=a, B_{y}=b\right)$ obtained when using the optimal CGLMP measurements on $\left|\psi^{+}\right\rangle$have several symmetries, detailed in Appendix A. For instance, they only depend on the difference $a-b=k \bmod d$. If we impose that our Bell expressions respect this particular symmetry, the probabilities $P\left(A_{x}=j+k \bmod d, B_{y}=j\right)$ should be treated equally for all $j$. In other words, the Bell expressions should be written as linear combinations of $P\left(A_{x}=B_{y}+k\right):=\sum_{j=0}^{d-1} P\left(A_{x}=j+k \bmod d, B_{y}=j\right)$. Taking into account the other symmetries (see Appendix A), a generic form for our Bell expressions is

$$
\begin{equation*}
I_{d, m}:=\sum_{k=0}^{\lfloor d / 2\rfloor-1}\left(\alpha_{k} \mathbb{P}_{k}-\beta_{k} \mathbb{Q}_{k}\right) \tag{6}
\end{equation*}
$$

where

$$
\begin{equation*}
\mathbb{P}_{k}:=\sum_{i=1}^{m}\left[P\left(A_{i}=B_{i}+k\right)+P\left(B_{i}=A_{i+1}+k\right)\right] \tag{7}
\end{equation*}
$$

and

$$
\begin{equation*}
\mathbb{Q}_{k}:=\sum_{i=1}^{m}\left[P\left(A_{i}=B_{i}-k-1\right)+P\left(B_{i}=A_{i+1}-k-1\right)\right] \tag{8}
\end{equation*}
$$

and where we define that $A_{m+1}:=A_{1}+1$. The parameters $\alpha_{k}$ and $\beta_{k}$ are the only degrees of freedom left and we fix them such that the resulting Bell inequalities are indeed maximally violated by the state $\left|\psi^{+}\right\rangle$. Note that taking $\alpha_{k}=\beta_{k}=1-2 k /(d-1)$ for $m=2$, one recovers the CGLMP Bell inequalities.

To exploit the symmetries inherent in Bell inequalities, we often write them in terms of correlators instead of probabilities. For two-output measurements one can switch from correlators to probabilities by means of an invertible transformation, but for $d>2$ it becomes necessary to appeal to the notion of generalized correlators. These are in general complex numbers
that are defined through the two-dimensional discrete Fourier transform of the probabilities $P\left(A_{x}=a, B_{y}=b\right)$, that is,

$$
\begin{equation*}
\left\langle A_{x}^{k} B_{y}^{l}\right\rangle=\sum_{a, b=0}^{d-1} \omega^{a k+b l} P\left(A_{x}=a, B_{y}=b\right) \tag{9}
\end{equation*}
$$

where $\omega=\exp (2 \pi i / d)$ and $k, l \in\{0, \ldots, d-1\}$, and $\left\{A_{x}^{k}\right\}_{k}$ and $\left\{B_{y}^{l}\right\}_{l}$ can be thought of as measurements whose outcomes are labelled by roots of unity $\omega^{i}(i=0, \ldots, d-1)$. For quantum correlations these numbers can be expressed in terms of the Born's rule. Indeed, assuming correlations $\vec{p}$ to be quantum and given by Eq. (2), we can interpret $\left\langle A_{x}^{k} B_{y}^{l}\right\rangle$ as the average value of the tensor product of the following operators

$$
\begin{equation*}
A_{x}^{k}=\sum_{a=0}^{d-1} \omega^{a k} P_{a}^{(x)} \quad \text { and } \quad B_{y}^{l}=\sum_{b=0}^{d-1} \omega^{b l} P_{b}^{(y)} \tag{10}
\end{equation*}
$$

in the state $|\psi\rangle$. Thus, in what follows, whenever we work with quantum correlations we have the above representation in mind. Note the operators in Eq. (10) are unitary, their eigenvalues are the roots of unity, and they enjoy properties such as $\left(A_{x}^{k}\right)^{\dagger}=A_{x}^{d-k}$ and $\left(B_{y}^{l}\right)^{\dagger}=B_{y}^{d-l}$ for any $k, l=0, \ldots, d-1$.

Exploiting now transformation (9), expression (6) can be rewritten as

$$
\begin{equation*}
\widetilde{I}_{d, m}=\sum_{i=1}^{m} \sum_{l=1}^{d-1}\left\langle A_{i}^{l} \bar{B}_{i}^{l}\right\rangle \tag{11}
\end{equation*}
$$

where, for clarity, the change of variables $\bar{B}_{i}^{l}=a_{l} B_{i}^{d-l}+a_{l}^{*} B_{i-1}^{d-l}$ with $a_{l}=\sum_{k=0}^{\lfloor d / 2\rfloor-1}\left(\alpha_{k} \omega^{-k l}-\right.$ $\beta_{k} \omega^{(k+1) l}$ ) was introduced on Bob's side. Note that due to the convention $A_{m+1}=A_{1}+1$, the term $\bar{B}_{1}^{l}$ is defined in a slightly different manner as $\bar{B}_{1}^{l}=a_{l} B_{1}^{d-l}+a_{l}^{*} \omega^{l} B_{m}^{d-l}$. For simplicity, we ignored an irrelevant scalar term in (11) and rescaled the expression. To recover $I_{d, m}$ exactly from $\widetilde{I}_{d, m}$, one has to add that scalar term corresponding to $l=0$, and divide the expression by $d$.

Each choice for the free parameters $\alpha_{k}$ and $\beta_{k}$ now corresponds to a choice for the variables $\bar{B}_{i}^{l}$. As explained above, our aim is to fix their value according to the quantum property we need: maximal violation by the maximally entangled state $\left|\psi^{+}\right\rangle$. At this point, it is instructive to look at the specific example of the CHSH Bell expression $(m=2, d=2)$. In the notation (11), we write the CHSH Bell expression $\left\langle A_{1} B_{1}\right\rangle+\left\langle A_{1} B_{2}\right\rangle+\left\langle A_{2} B_{1}\right\rangle-\left\langle A_{2} B_{2}\right\rangle$ as

$$
\begin{equation*}
\tilde{I}_{2,2}=\left\langle A_{1} \bar{B}_{1}\right\rangle+\left\langle A_{2} \bar{B}_{2}\right\rangle \tag{12}
\end{equation*}
$$

where $\bar{B}_{1}=\left(B_{1}+B_{2}\right) / \sqrt{2}$ and $\bar{B}_{2}=\left(B_{1}-B_{2}\right) / \sqrt{2}$. Notice now that for the optimal measurements leading to the quantum bound of the CHSH inequality, we have that $\bar{B}_{1}=A_{1}^{*}$ and $\bar{B}_{2}=A_{2}^{*}$. Our intuition is to fix this condition generically for any $m$ and $d$ : we choose the parameters $\alpha_{k}$ and $\beta_{k}$ such that the conditions

$$
\begin{equation*}
\bar{B}_{i}^{l}=\left(A_{i}^{l}\right)^{*} \tag{13}
\end{equation*}
$$

hold for $l=1, \ldots, d-1$ and $i=1, \ldots, m$, in the case that the initial operators $\left\{P_{a}^{(x)}\right\}$ and $\left\{P_{b}^{(y)}\right\}$ are the optimal CGLMP operators. Further intuition for imposing these exact conditions will be provided in the next section, where we prove the Tsirelson bound of the expressions.

Conditions (13) give rise to a set of linear equations for the variables $\alpha_{k}$ and $\beta_{k}$ which is solved in detail in Appendix B, giving

$$
\begin{gather*}
\alpha_{k}=\frac{1}{2 d} \tan \left(\frac{\pi}{2 m}\right)[g(k)-g(\lfloor d / 2\rfloor)]  \tag{14}\\
\beta_{k}=\frac{1}{2 d} \tan \left(\frac{\pi}{2 m}\right)\left[g\left(k+1-\frac{1}{m}\right)+g(\lfloor d / 2\rfloor)\right] \tag{15}
\end{gather*}
$$

with $g(x):=\cot \left(\pi\left(x+\frac{1}{2 m}\right) / d\right)$.
To sum up, our class of Bell expressions is given by $I_{d, m}$ (6) or equivalently by $\widetilde{I}_{d, m}$ (11), with coefficients (14) and (15). We arrived at this class of Bell expressions by first writing the most general Bell expression satisfying the symmetry of CGLMP correlations, then re-writing these Bell expressions in the simple form (11) through a change of variable on Bob's side, and then imposing the conditions (13) that generalize a property observed in the CHSH case. So far we cannot guarantee that these Bell expressions lead to proper Bell inequalities violated by quantum theory, nor that their quantum bound is attained by the maximally entangled state $\left|\psi^{+}\right\rangle$, but we show in the next section that this is indeed the case.

## 4 Properties of the novel Bell expressions

We now present our main results for the class of Bell expressions (11). All the values for the bounds of (6) can be obtained directly from those of (11) as mentioned in Appendix B.

Theorem 1. The classical bound of $\widetilde{I}_{d, m}$ is given by

$$
\begin{equation*}
\widetilde{C}_{b}=\frac{1}{2} \tan \left(\frac{\pi}{2 m}\right)\left\{(2 m-1) \cot \left(\frac{\pi}{2 d m}\right)-\cot \left[\frac{\pi}{d}\left(1-\frac{1}{2 m}\right)\right]\right\}-m \tag{16}
\end{equation*}
$$

Proof. We start with the probability version $I_{d, m}$ of the Bell expression, and since we can restrict the problem to local deterministic strategies, finding the classical bound becomes a question of distributing 1s and 0 s over all the terms $P\left(A_{x}=B_{y}+z\right)$. It turns out that the maximizing strategy is to have $2 m-1$ terms equal to 1 multiplied by $\alpha_{0}$ and 1 term equal to 1 multiplied by $\beta_{0}$. All other terms must be equal to 0 . More details can be found in Appendix C .

Importantly, the resulting Bell inequality $\widetilde{I}_{d, m} \leq \widetilde{C}_{b}$ is violated by quantum mechanics. Indeed, we can reach the value $m(d-1)$ for $\widetilde{I}_{d, m}$ by applying the CGLMP measurements on the maximally entangled state. This is easily seen using Eq. (13), the unitarity of $A_{i}^{k}$, and the following property of the maximally entangled states: $M \otimes N\left|\psi^{+}\right\rangle=\mathbb{I} \otimes N M^{T}\left|\psi^{+}\right\rangle$for $M$ and $N$ operators. One can see how all the correlators in (11) are then equal to 1 , yielding the quantum violation of $m(d-1)$ after summing over $i$ and $l$.

Crucially, as we prove below, the value $m(d-1)$ turns out to be the maximal quantum violation of our Bell inequalities.
Theorem 2. The Tsirelson bound of $\widetilde{I}_{d, m}$ is given by $\widetilde{Q}_{b}=m(d-1)$.
Proof. Here we present a sketch of the proof, while its more detailed version is deferred to Appendix D. The idea of the proof is to construct a sum-of-squares (SOS) decomposition of the shifted Bell operator $\widetilde{\mathcal{B}}:=\widetilde{Q}_{b} \mathbb{I}-\mathcal{B}$, where $\mathbb{I}$ is the identity operator and $\mathcal{B}$ the Bell operator corresponding to expression (11), as was done for instance in [25]. For any positive semidefinite operator $\mathcal{P}$, an SOS decomposition is a finite collection of operators $P_{\lambda}$ such that

$$
\begin{equation*}
\mathcal{P}=\sum_{\lambda} P_{\lambda}^{\dagger} P_{\lambda} \tag{17}
\end{equation*}
$$

It is clear that if the shifted Bell operator $\widetilde{\mathcal{B}}$ can be written as (17) it must be semidefinite positive, which proves that $\widetilde{Q}_{b}$ is an upper bound to our Bell expression. Indeed, for any quantum state $|\psi\rangle$, it then holds that $\langle\psi| \widetilde{\mathcal{B}}|\psi\rangle \geq 0$, which implies for the Bell operator that $\langle\psi| \mathcal{B}|\psi\rangle \leq \widetilde{Q}_{b}$. This approach is in principle valid for any shifted Bell operator, thus for any Bell expression. As we expect the $P_{\lambda}$ 's to be polynomials of the measurement operators of Alice and Bob, we can define the order of the SOS decomposition as the largest degree of these polynomials.

In our case, we show that $\widetilde{Q}_{b}=m(d-1)$ is indeed the maximal quantum violation of our class of Bell inequalities as the shifted Bell operator $\widetilde{Q}_{b} \mathbb{1}-\mathcal{B}$ can be decomposed as

$$
\begin{equation*}
\widetilde{Q}_{b} \mathbb{1}-\mathcal{B}=\frac{1}{2} \sum_{i=1}^{m} \sum_{k=1}^{d-1} P_{i k}^{\dagger} P_{i k}+\frac{1}{2} \sum_{i=1}^{m-2} \sum_{k=1}^{d-1} T_{i k}^{\dagger} T_{i k}, \tag{18}
\end{equation*}
$$

where $P_{i k}=\mathbb{1} \otimes \bar{B}_{i}^{k}-\left(A_{i}^{k}\right)^{\dagger} \otimes \mathbb{1}$, and $T_{i k}=\left(\mu_{i, k} B_{2}^{d-k}+\nu_{i, k} B_{i+2}^{d-k}+\tau_{i, k} B_{i+3}^{d-k}\right)$ with $\mu_{i, k}, \nu_{i, k}$, $\tau_{i, k} \in \mathbb{R}$. Our Bell operator is $\mathcal{B}=\sum_{i=1}^{m} \sum_{l=1}^{d-1} A_{i}^{k} \otimes \bar{B}_{i}^{k}$, and the decomposition is independent of the choice of $A_{i}^{k}$ and $B_{i}^{k}$. The second sum of terms with coefficients $\mu_{i, k}, \nu_{i, k}$ and $\tau_{i, k}$ was added to compensate some non-vanishing terms in the first sum. The exact values of the coefficients along with details on the SOS decomposition can be found in Appendix D.

Let us elaborate on how the SOS works in the case $m=2$, which justifies a posteriori the imposition of conditions (13). For $m=2$, only the first part of the SOS decomposition (18) remains. At the point of maximal violation, both sides of (18) applied on $\left|\psi^{+}\right\rangle$must yield 0 . Since the measurements are now the optimal CGLMP ones, Eq. (13) holds, and can be used as above with the property $M \otimes N\left|\psi^{+}\right\rangle=\mathbb{1} \otimes N M^{T}\left|\psi^{+}\right\rangle$to see easily how the first sum of the decomposition cancels. One can now grasp the intuition behind conditions (13): imposing them leads to having an SOS of the form (18), more precisely an SOS of order one in the operators $A_{i}^{k}$ and $B_{i}^{k}$.

In the CHSH case, one can observe the same effect, as these same properties of the optimal state and measurements allow the Bell operator $\mathcal{B}_{\text {CHSH }}=A_{1} \otimes B_{1}+A_{1} \otimes B_{2}+A_{2} \otimes B_{1}-A_{2} \otimes B_{2}$ to have the following SOS decomposition, which is also of order one:

$$
\begin{equation*}
2 \sqrt{2} \mathbb{1}-\mathcal{B}_{\mathrm{CHSH}}=\frac{1}{\sqrt{2}}\left(P_{1}^{\dagger} P_{1}+P_{2}^{\dagger} P_{2}\right) \tag{19}
\end{equation*}
$$

with $P_{1}=(1 / \sqrt{2})\left(\mathbb{1} \otimes B_{1}+\mathbb{1} \otimes B_{2}\right)-A_{1} \otimes \mathbb{1}$, and $P_{2}=(1 / \sqrt{2})\left(\mathbb{1} \otimes B_{1}-\mathbb{1} \otimes B_{2}\right)-A_{2} \otimes \mathbb{1}$. Thus, our construction generalizes this quantum aspect of CHSH. In the case $m>2$, the SOS does not generalize as directly, and one has to add "by hand" the extra terms $T_{i k}^{\dagger} T_{i k}$. However, the order of the SOS remains one.

Theorem 3. The no-signalling bound of $\widetilde{I}_{d, m}$ is given by

$$
\begin{equation*}
\widetilde{N S}_{b}=m \tan \left(\frac{\pi}{2 m}\right) \cot \left(\frac{\pi}{2 d m}\right)-m \tag{20}
\end{equation*}
$$

Proof. In Appendix E, we provide a no-signalling behaviour and show that it attains the algebraic bound of our Bell expressions. It corresponds to having all the probabilities which are multiplied by $\alpha_{0}$ in $I_{d, m}$ equal to 1 , and all the others equal to 0 .

For our expressions to form a non-trivial Bell inequalities, the classical bound must be smaller than the quantum one for all $m, d \geq 2$. We show this in Appendix F, and we also study the scaling of the classical, quantum, and no-signalling bounds.

Finally, note that for $m=2$, our Bell expressions coincide with those introduced in Refs. [26] and then rederived in [27] using a different approach. Moreover, the maximal quantum violations of these Bell inequalities was computed in Refs. [28, 27] exploiting alternative techniques. On the other hand, for $d=2$ and any $m$, our class recovers the well-known chained Bell inequalities [29].

## 5 Applications to device-independent protocols

A natural application for our expressions is self-testing, a DI protocol in which a state and measurements performed on it are certified up to local isometries, based on the nonlocal correlations they produce - here, on the violation of a Bell inequality. To perform self-testing, the point of maximal violation must be unique, which is a property that we have not proven for our inequalities. There exists a numerical method for self-testing called the SWAP method [30], and we applied it to the simplest case $m=2$ and $d=3$. The results of the program are plotted in Figure 1. It shows that, in this scenario, the maximal violation is unique and self-testing the maximally entangled state of two qutrits $\left|\psi^{+}\right\rangle=\frac{1}{\sqrt{3}}(|00\rangle+|11\rangle+|22\rangle)$ is possible, with robustness.

An open question consists in generalizing these self-testing results to any dimension, which must be done analytically. Our inequalities could then find a direct application in DI random number generation protocols [5, 6, 31]. Indeed, if the point of maximal violation is proven to be unique, one can successfully apply the method of [32] and use the symmetries of the Bell expressions to guarantee a dit of randomness when observing the maximal violation. Ultimately, by increasing the dimension $d$, one would achieve unbounded randomness expansion.

Our inequalities could also find applications in DI quantum key distribution. Indeed, it was shown in [33] through the example of the CGLMP inequalities that exploiting high dimensional systems can be beneficial in noisy scenarios. An advantage that our inequalities have over CGLMP in that scenario is that the maximally entangled state can produce perfect correlations between the users, which should lead to higher key generation rates than using the CGLMP inequalities.


Figure 1: Minimum fidelity of state in the black box to the maximally entangled state of two qutrits, as a function of the violation of a renormalised version of $I_{3,2}$. At the maximal violation $2+2 / \sqrt{3}$, the fidelity is equal to 1 , meaning that the quantum state used in the Bell experiment must be equal to the reference state. For lower violations, the fidelity decreases.

## 6 Discussion

In summary, we have introduced a new technique allowing to construct Bell inequalities with an arbitrary number of measurements and outcomes that are maximally violated by the maximally entangled states. It exploits the concept of SOS decompositions of Bell operators and, crucially, allows one to compute analytically their Tsirelson bounds. We also provide the classical and no-signalling bounds of the resulting Bell inequalities. Our results are very general as, unlike previous works, we do not consider a particular Bell scenario, but allow the number of inputs $m$ and outputs $d$ to be arbitrary. Our inequalities can be seen as the "quantum" or the DI-oriented generalization of CHSH Bell inequality in the same spirit as the CGLMP inequality generalizes the CHSH one classically. Indeed, while the CGLMP inequalities preserve the property of being facets of the local polytope, our inequalities possess the same sum-of-squares structure as CHSH at the maximal quantum violation, which leads to the important property for DI protocols of being maximally violated by the maximal entangled state.

Moreover, let us note that deriving Tsirelson bounds allows us to gain insight about the quantum set of correlations - more specifically its boundary - and has thus fundamental implications. In particular, a feature of our class of inequalities worth highlighting is that their Tsirelson bound corresponds to the bound obtained using the NPA hierarchy at the first level, i.e., within the set $\mathcal{Q}_{1}$. This is a rare property, which to our knowledge has been previously observed only for XOR games. That the Tsirelson bounds of our inequalities are attained in $\mathcal{Q}_{1}$ follows from our SOS decomposition (see Eq. (18)). Indeed the degree of an optimal SOS decomposition for a Bell operator is directly linked to the level of the NPA hierarchy at which the quantum bound is obtained [34]. An SOS of degree 1, as in our case, corresponds to the first level $\mathcal{Q}_{1}$.

This means that the boundaries of the sets $\mathcal{Q}$ and $\mathcal{Q}_{1}$ intersect on the point of maximal violation of our inequalities. This observation, in conjunction with the results of Ref. [27], raises a question about $\mathcal{Q}_{1}$. Indeed, the boundaries of $\mathcal{Q}$ and $\mathcal{Q}_{1}$ seems to intersect at points that correspond to the maximal violation of Bell inequalities attained by maximally entangled states. One should confirm whether this trend is a general property, and could perhaps use it as a way to characterize $\mathcal{Q}_{1}$.

## Acknowledgments

We wish to thank M. Navascués and T. Vértesi for fruitful discussions, and especially J.D. Bancal for sharing with us his code. This work was supported ERC CoG QITBOX and AdG OSYRIS, the AXA Chair in Quantum Information Science, Spanish MINECO (FOQUS FIS2013-46768-P and SEV-2015-0522), Fundació Privada Cellex, the Generalitat de Catalunya (SGR 874 and SGR 875), the EU projects QALGO and SIQS, and the John Templeton Foundation. S. P. is a Research Associate of the Fonds de la Recherche Scientifique F.R.S.-FNRS (Belgium). R. A. acknowledges funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 705109.

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## A Optimal CGLMP measurements

We present here the "optimal CGLMP measurements" first introduced in [22] and generalized to an arbitrary number of inputs in [23]. We use them throughout our work. They are defined as follows

$$
\begin{equation*}
A_{x}=U_{x}^{\dagger} F \Omega F^{\dagger} U_{x}, \quad B_{y}=V_{y} F^{\dagger} \Omega F V_{y}^{\dagger} \tag{21}
\end{equation*}
$$

where $\Omega=\operatorname{diag}\left[1, \omega, \omega^{2}, \ldots, \omega^{d-1}\right]$, with $\omega=\exp (2 \pi i / d)$, and $F$ is the $d \times d$ discrete Fourier transform matrix given by

$$
\begin{equation*}
F_{d}=\frac{1}{\sqrt{d}} \sum_{i, j=0}^{d-1} \omega^{i j}|i\rangle\langle j| . \tag{22}
\end{equation*}
$$

Then, $U_{x}$ and $V_{x}$ are unitary operations defining Alice's and Bob's measurements and read explicitly

$$
\begin{equation*}
U_{x}=\sum_{j=0}^{d-1} \omega^{j \theta_{x}}|j\rangle\langle j|, \quad V_{y}=\sum_{j=0}^{d-1} \omega^{j \zeta_{y}}|j\rangle\langle j| \tag{23}
\end{equation*}
$$

with the phases $\theta_{x}=(x-1 / 2) / m$ and $\zeta_{y}=y / m$ for $x, y=1, \ldots, m$.
When applying these measurements on a normalised state of the form $|\psi\rangle=\sum_{q=0}^{d-1} \gamma_{q}|q q\rangle$, we obtain the probabilities

$$
\begin{equation*}
P\left(A_{x}=a, B_{y}=b\right)=\left|\frac{1}{d} \sum_{q=0}^{d-1} \gamma_{q} \exp \left(\frac{2 \pi i}{d} q\left(a-b-\theta_{x}+\zeta_{y}\right)\right)\right|^{2} . \tag{24}
\end{equation*}
$$

One can observe that this depends only on the difference $k=a-b$ and not on $a$ and $b$ separately. This means that:

$$
\begin{equation*}
P\left(A_{x}=B_{y}+k\right)=d P\left(A_{x}=k, B_{y}=0\right) . \tag{25}
\end{equation*}
$$

Thus, all the terms $P\left(A_{x}=B_{y}+k\right)$ appearing in the inequalities (6) computed for those measurements and state have identical subterms $P\left(A_{x}=b+k, B_{y}=b\right)$. Moreover, using the values of the phases $\theta_{x}$ and $\zeta_{y}$, one can verify straightforwardly that expression (24) has the same value if $x=y$ and $a-b=k$, and if $x=y+1$ and $a-b=-k$. Thus :

$$
\begin{equation*}
P\left(A_{i}=B_{i}+k\right)=P\left(B_{i}=A_{i+1}+k\right), \tag{26}
\end{equation*}
$$

for $i=1, \ldots, m$. Note that if one wants to replace $A_{m+1}=A_{1}$, the symmetry is not valid anymore and requires the definition $A_{m+1}=A_{1}+1$, which we adopt. To sum up, all the $\mathbb{P}_{k}$ and $\mathbb{Q}_{k}$ appearing in (6) have identical subterms for those state and optimal CGLMP measurements (in particular the state can be the maximally entangled state). These symmetries justify the form of the Bell expressions (6): terms who have the same value appear with the same coefficient $\alpha_{k}$ or $\beta_{k}$, thus forming "blocks". Different blocks have different values and are multiplied by different coefficients.

## B Derivation of coefficients $\alpha_{k}$ and $\beta_{k}$

We present the details on the derivation of coefficients (14) and (15). The departure point of the determination of $\alpha_{k}$ and $\beta_{k}$ is the set of matrix conditions (13) which we restate explicitly here

$$
\begin{equation*}
\bar{B}_{i}^{l}=\left(A_{i}^{l}\right)^{*} \tag{13}
\end{equation*}
$$

with $i=1, \ldots, m$, and $l=1, \ldots,\lfloor d / 2\rfloor$. This number $\lfloor d / 2\rfloor$ of equations stems from the fact that $A_{x}^{d-l}=\left(A_{x}^{l}\right)^{\dagger}$ and $\bar{B}_{y}^{d-l}=\left(\bar{B}_{y}^{l}\right)^{\dagger}$. Recall that the barred quantities $\bar{B}_{i}^{l}$ are defined as

$$
\begin{equation*}
\bar{B}_{i}^{l}=a_{l} B_{i}^{d-l}+a_{l}^{*} B_{i-1}^{d-l} \tag{27}
\end{equation*}
$$

for $i=2, \ldots, m$ and $\bar{B}_{1}^{l}=a_{l} B_{1}^{d-l}+a_{l}^{*} \omega^{l} B_{m}^{d-l}$, and the numbers $a_{l}$ are given by

$$
\begin{equation*}
a_{l}=\sum_{k=0}^{\lfloor d / 2\rfloor-1}\left[\alpha_{k} \omega^{-k l}-\beta_{k} \omega^{(k+1) l}\right] . \tag{28}
\end{equation*}
$$

In order to solve the system (13) one has to find explicit forms of $A_{x}^{l}$ and $B_{y}^{l}$. Introducing Eqs. (22) and (23) into Eq. (21), one obtains

$$
\begin{equation*}
A_{x}^{l}=\omega^{-(d-l) \theta_{x}} \sum_{n=0}^{l-1}|d-l+n\rangle\langle n|+\omega^{l \theta_{x}} \sum_{n=l}^{d-1}|n-l\rangle\langle n| \tag{29}
\end{equation*}
$$

and

$$
\begin{equation*}
B_{y}^{l}=\omega^{-(d-l) \zeta_{y}} \sum_{n=0}^{l-1}|n\rangle\langle d-l+n|+\omega^{l \zeta \zeta_{y}} \sum_{n=l}^{d-1}|n\rangle\langle n-l| . \tag{30}
\end{equation*}
$$

Then, one combines these formulas with equations (27) and (13), and compares the matrix elements, which yields the following system of equations

$$
\begin{align*}
a_{l} \omega^{-l \zeta_{i}}+a_{l}^{*} \omega^{-l \zeta_{i-1}} & =\omega^{-l \theta_{i}} \\
a_{l} \omega^{(d-l) \zeta_{i}}+a_{l}^{*} \omega^{(d-l) \zeta_{i-1}} & =\omega^{(d-l) \theta_{i}}, \tag{31}
\end{align*}
$$

with $i=1, \ldots, m$ and $l=1, \ldots,\lfloor d / 2\rfloor$, where it is assumed that $\zeta_{0}=0$. Simple algebra implies finally that

$$
\begin{equation*}
a_{l}=\frac{\omega^{\frac{2 l-d}{4 m}}}{2 \cos (\pi / 2 m)} \quad(l=1, \ldots,\lfloor d / 2\rfloor) \tag{32}
\end{equation*}
$$

Having determined $a_{l}$, one can turn to the system (28). It consists of $\lfloor d / 2\rfloor$ equations containing $2\lfloor d / 2\rfloor$ variables, meaning that it cannot be uniquely solved, and, in particular, the solutions will be generally complex. To handle the latter problem we equip this system with $\lfloor d / 2\rfloor$ additional equations

$$
\begin{equation*}
\sum_{k=0}^{\lfloor d / 2\rfloor-1}\left[\alpha_{k} \omega^{k l}-\beta_{k} \omega^{-(k+1) l}\right]=a_{l}^{*} . \tag{33}
\end{equation*}
$$

for $l=1, \ldots,\lfloor d / 2\rfloor$. Now, both systems (28) and (33) can be condensed into the following single one

$$
\begin{equation*}
\sum_{k=0}^{\lfloor d / 2\rfloor-1}\left[\alpha_{k} \omega^{-k l}-\beta_{k} \omega^{(k+1) l}\right]=c_{l} \tag{34}
\end{equation*}
$$

in which $c_{l}=a_{l}$ for $l=1, \ldots,\lfloor d / 2\rfloor$ and $c_{l}=c_{-l}^{*}$ for $l=-\lfloor d / 2\rfloor, \ldots,-1$. In what follows we solve (33) for even and odd $d$ separately.

Odd $d$. We begin by noting that in this case, the system (34) consists of $d-1$ equations and involves the same number of variables, and therefore one expects it to have a unique solution. To find it, we denote the set $I:=\{-(d-1) / 2, \ldots,-1,1, \ldots,(d-1) / 2\}$ and note that for any pair $k, n \in\{0, \ldots,\lfloor d / 2\rfloor-1\}$, the following identity holds:

$$
\begin{equation*}
\sum_{l \in I} \omega^{-l k} \omega^{l n}=\sum_{l \in I \cup\{0\}} \omega^{-l k} \omega^{l n}-1=d \delta_{n, k}-1 \tag{35}
\end{equation*}
$$

We then multiply (34) by $\omega^{n l}$ for some $n \in\{0, \ldots,\lfloor d / 2\rfloor-1\}$ and add the resulting equations over $l \in I$, which by virtue of Eq. (35) gives

$$
\begin{equation*}
\alpha_{n}=\frac{1}{d} S+\frac{1}{d} \sum_{l \in I} c_{l} \omega^{n l} \quad(n=0, \ldots,\lfloor d / 2\rfloor-1) \tag{36}
\end{equation*}
$$

where we have denoted

$$
\begin{equation*}
S=\sum_{k=0}^{\lfloor d / 2\rfloor-1}\left(\alpha_{k}-\beta_{k}\right) \tag{37}
\end{equation*}
$$

The coefficients $\beta_{n}$ can be determined in an analogous way and we obtain:

$$
\begin{equation*}
\beta_{n}=-\frac{1}{d} S-\frac{1}{d} \sum_{l \in I} c_{l} \omega^{-(n+1) l} \quad(n=0, \ldots,\lfloor d / 2\rfloor-1) \tag{38}
\end{equation*}
$$

To fully determine $\alpha_{n}$ and $\beta_{n}$, it is in fact enough to compute the sum in Eq. (36) as the second one and $S$ can be obtained from it by replacing $n$ by $-(n+1)$ and $\lfloor d / 2\rfloor$, respectively. To compute this sum, we first express it as

$$
\begin{align*}
\sum_{l \in I} c_{l} \omega^{n l} & =\frac{1}{\cos (\pi / 2 m)} \sum_{l=1}^{\lfloor d / 2\rfloor} \operatorname{Re}\left(\omega^{(2 l-d) / 4 m} \omega^{n l}\right) \\
& =\frac{1}{\cos (\pi / 2 m)}\left[\cos \left(\frac{\pi}{2 m}\right) \sum_{l=1}^{\lfloor d / 2\rfloor} \cos \left(\frac{2 \pi l}{d} \xi\right)+\sin \left(\frac{\pi}{2 m}\right) \sum_{l=1}^{\lfloor d / 2\rfloor} \sin \left(\frac{2 \pi l}{d} \xi\right)\right] \tag{39}
\end{align*}
$$

where we have denoted $\xi=n+1 / 2 m$. Using the Euler representations of the cosine and sine functions the above two sums can be easily computed and they read

$$
\begin{equation*}
\sum_{l=1}^{\lfloor d / 2\rfloor} \cos \left(\frac{2 \pi l}{d} \xi\right)=\frac{1}{2}\left[\frac{\sin (\pi \xi)}{\sin (\pi \xi / d)}-1\right] \tag{40}
\end{equation*}
$$

and

$$
\begin{equation*}
\sum_{l=1}^{\lfloor d / 2\rfloor} \sin \left(\frac{2 \pi l}{d} \xi\right)=\frac{1}{2}\left[\cot \left(\frac{\pi \xi}{d}\right)-\frac{\cos (\pi \xi)}{\sin (\pi \xi / d)}\right] \tag{41}
\end{equation*}
$$

Introducing them into Eq. (39) and with the aid of some trigonometric formulas, one obtains

$$
\begin{align*}
\sum_{l \in I} c_{l} \omega^{n l} & =\frac{1}{2}\left\{\frac{\sin (\pi \xi)}{\sin (\pi \xi / d)}-1+\tan \left(\frac{\pi}{2 m}\right)\left[\cot \left(\frac{\pi \xi}{d}\right)-\frac{\cos (\pi \xi)}{\sin (\pi \xi / d)}\right]\right\} \\
& =\frac{1}{2}\left\{\tan \left(\frac{\pi}{2 m}\right) \cot \left[\frac{\pi}{d}\left(n+\frac{1}{2 m}\right)\right]-1\right\} \tag{42}
\end{align*}
$$

By replacing $n$ with $-(n+1)$ in the above formula we then arrive at the expression for the sum in Eq. (38), that is,

$$
\begin{equation*}
\sum_{l \in I} c_{l} \omega^{-(n+1) l}=-\frac{1}{2}\left\{\tan \left(\frac{\pi}{2 m}\right) \cot \left[\frac{\pi}{d}\left(n+1-\frac{1}{2 m}\right)\right]+1\right\} \tag{43}
\end{equation*}
$$

Finally, setting $n=\lfloor d / 2\rfloor=(d-1) / 2$ in Eq. (42) one obtains a formula for $S$ :

$$
\begin{equation*}
S=\frac{1}{2}\left\{1-\tan \left(\frac{\pi}{2 m}\right) \cot \left[\frac{\pi}{d}\left(\left\lfloor\frac{d}{2}\right\rfloor+\frac{1}{m}\right)\right]\right\} . \tag{44}
\end{equation*}
$$

Substituting Eqs. (42), (43), and (44) into Eqs. (36) and (38), we eventually obtain the coefficients $\alpha_{n}$ and $\beta_{n}$ in the following form

$$
\begin{equation*}
\alpha_{n}=\frac{1}{2 d} \tan \left(\frac{\pi}{2 m}\right)\left\{\cot \left[\frac{\pi}{d}\left(n+\frac{1}{2 m}\right)\right]-\cot \left[\frac{\pi}{d}\left(\left\lfloor\frac{d}{2}\right\rfloor+\frac{1}{2 m}\right)\right]\right\} \tag{45}
\end{equation*}
$$

and

$$
\begin{equation*}
\beta_{n}=\frac{1}{2 d} \tan \left(\frac{\pi}{2 m}\right)\left\{\cot \left[\frac{\pi}{d}\left(n+1-\frac{1}{2 m}\right)\right]+\cot \left[\frac{\pi}{d}\left(\left\lfloor\frac{d}{2}\right\rfloor+\frac{1}{2 m}\right)\right]\right\} \tag{46}
\end{equation*}
$$

with $n=1, \ldots,\lfloor d / 2\rfloor$. As in the main text, the coefficients can be expressed using function $g(x):=\cot \left(\frac{\pi}{d}\left(x+\frac{1}{2 m}\right)\right)$.

Even $d$. Clearly, in the case of even $d$, one can solve the system (34) analogously. The difference is, however, that (34) is the same equation for $l=-d / 2$ and $l=d / 2$, and therefore the system consists of $d-1$ equations for $d$ variables. A non-unique solution is then expected.

Denoting $I_{e}=\{-(d-1) / 2, \ldots,-1,1, \ldots, d / 2\}$ and following the same methodology as above with the set $I$ replaced by $I_{e}$ one arrives at $\alpha_{n}$ and $\beta_{n}$ given by

$$
\begin{equation*}
\alpha_{n}=\frac{1}{2 d}\left\{\tan \left(\frac{\pi}{2 m}\right) \cot \left[\frac{\pi}{d}\left(n+\frac{1}{2 m}\right)\right]-1\right\}+\frac{1}{d} S \tag{47}
\end{equation*}
$$

and

$$
\begin{equation*}
\beta_{n}=\frac{1}{2 d}\left\{\tan \left(\frac{\pi}{2 m}\right) \cot \left[\frac{\pi}{d}\left(n+1-\frac{1}{2 m}\right)\right]+1\right\}-\frac{1}{d} S \tag{48}
\end{equation*}
$$

where $S$ is given by the same formula as in Eq. (37). Here, the quantity $S$ (or, equivalently, one of the variables $\alpha_{n}$ or $\beta_{n}$ ) cannot be uniquely determined. We fix it in such a way that the resulting $\alpha_{n}$ and $\beta_{n}$ are given by the same formulas as those in the odd $d$ case, that is,

$$
\begin{equation*}
S=\frac{1}{2}\left\{1-\tan \left(\frac{\pi}{2 m}\right) \cot \left[\frac{\pi}{d}\left(\left\lfloor\frac{d}{2}\right\rfloor+\frac{1}{2 m}\right)\right]\right\} \tag{49}
\end{equation*}
$$

As a consequence the coefficients $\alpha_{n}$ and $\beta_{n}$ are given by Eqs. (45) and (46), both in the odd and even $d$ cases.

It is finally worth mentioning that the values of the two Bell expressions-in terms of probabilities (6) and in terms of generalized correlators (11)—are related in the following way:

$$
\begin{equation*}
\widetilde{I}_{d, m}=d I_{d, m}-2 m S \tag{50}
\end{equation*}
$$

where $S$ is given by equation (44).

Special cases. Let us now consider two special cases of $d=2$ and any $m$, and $m=2$ and any $d$. In the first one, the Bell expression in the probability form (6) simplifies to

$$
\begin{equation*}
I_{2, m}=\alpha_{0} \mathbb{P}_{0}-\beta_{0} \mathbb{Q}_{0} \tag{51}
\end{equation*}
$$

where

$$
\begin{equation*}
\mathbb{P}_{0}=\sum_{i=1}^{m}\left[P\left(A_{i}=B_{i}\right)+P\left(B_{i}=A_{i+1}\right)\right], \quad \mathbb{Q}_{0}=\sum_{i=1}^{m}\left[P\left(A_{i}=B_{i}-1\right)+P\left(B_{i}=A_{i+1}-1\right)\right] \tag{52}
\end{equation*}
$$

and

$$
\begin{equation*}
\alpha_{0}=\frac{1}{2 \cos (\pi / 2 m)}, \quad \beta_{0}=0 . \tag{53}
\end{equation*}
$$

Moreover, there is a unique coefficient $a_{1}$ and it simplifies to $1 /[2 \cos (\pi / 2 m)]$, so that in the correlator form our Bell expression for $d=2$ becomes

$$
\begin{equation*}
\widetilde{I}_{2, m}=\frac{1}{2 \cos (\pi / 2 m)}\left[\left\langle A_{1} B_{1}\right\rangle-\left\langle A_{1} B_{m}\right\rangle+\sum_{i=2}^{m}\left(\left\langle A_{i} B_{i}\right\rangle+\left\langle A_{i} B_{i-1}\right\rangle\right)\right], \tag{54}
\end{equation*}
$$

and Theorems 1, 2, and 3 give $\widetilde{C}_{b}=(m-1) / \cos [\pi / 2 m], \widetilde{Q}_{b}=m$, and $\widetilde{N S}_{b}=m / \cos [\pi / 2 m]$, respectively. This is the well-known chained Bell inequality [29], which was recently used in Ref. [35] to self-test the maximally entangled state of two qubits and the corresponding measurements.

In the second case, i.e., that of $m=2$ and any $d$, the Bell expression $I_{d, 2}$ in the probability form is given by Eq.

$$
\begin{equation*}
I_{d, 2}:=\sum_{k=0}^{\lfloor d / 2\rfloor-1}\left(\alpha_{k} \mathbb{P}_{k}-\beta_{k} \mathbb{Q}_{k}\right), \tag{55}
\end{equation*}
$$

with the expressions $\mathbb{P}_{k}$ and $\mathbb{Q}_{k}$ simplifying to

$$
\begin{equation*}
\mathbb{P}_{k}=P\left(A_{1}=B_{1}+k\right)+P\left(B_{1}=A_{2}+k\right)+P\left(A_{2}=B_{2}+k\right)+P\left(B_{2}=A_{1}+k+1\right) \tag{56}
\end{equation*}
$$

and

$$
\begin{equation*}
\mathbb{Q}_{k}=P\left(A_{1}=B_{1}-k-1\right)+P\left(B_{1}=A_{2}-k-1\right)+P\left(A_{2}=B_{2}-k-1\right)+P\left(B_{2}=A_{1}-k\right), \tag{57}
\end{equation*}
$$

where we have exploited the convention that $A_{3}=A_{1}+1$. Then, the coefficients $\alpha_{k}$ and $\beta_{k}$ are given by

$$
\begin{equation*}
\alpha_{k}=\frac{1}{2 d}\left[g(k)+(-1)^{d} \tan \left(\frac{\pi}{4 d}\right)\right], \quad \beta_{k}=\frac{1}{2 d}\left[g(k+1 / 2)-(-1)^{d} \tan \left(\frac{\pi}{4 d}\right)\right], \tag{58}
\end{equation*}
$$

with $g(k)=\cot [\pi(k+1 / 4) / d]$. On the other hand, in the correlator form one obtains

$$
\begin{equation*}
\widetilde{I}_{d, 2}=\sum_{l=1}^{d-1}\left[a_{l}\left\langle A_{1}^{l} B_{1}^{d-l}\right\rangle+a_{l}^{*} \omega^{l}\left\langle A_{1}^{l} B_{2}^{d-l}\right\rangle+a_{l}\left\langle A_{2}^{l} B_{2}^{d-l}\right\rangle+a_{l}^{*}\left\langle A_{2}^{l} B_{1}^{d-l}\right\rangle\right], \tag{59}
\end{equation*}
$$

where $a_{l}=\omega^{(2 l-d) / 8} / \sqrt{2}$. In this case Theorems 1,2 , and 3 give

$$
\begin{equation*}
\widetilde{C}_{b}=\frac{1}{2}\left[3 \cot \left(\frac{\pi}{3 d}\right)-\cot \left(\frac{3 \pi}{4 d}\right)\right]-2, \tag{60}
\end{equation*}
$$

$\widetilde{Q}_{b}=2(d-1)$, and $\widetilde{N S}_{b}=2 \cot [\pi /(4 d)]-2$. It should be noticed that this Bell inequality previously studied in Refs. [26] and [27], and, in particular in Ref. [27] and [28] the maximal quantum violation was found using two different methods.

## C Classical bound of the inequalities

Let us start with expression (6) and note that we can rewrite it as:

$$
\begin{equation*}
I_{d, m}:=\sum_{k=0}^{d-1} \alpha_{k} \sum_{i=1}^{m}\left[P\left(A_{i}=B_{i}+k\right)+P\left(B_{i}=A_{i+1}+k\right)\right], \tag{61}
\end{equation*}
$$

with $A_{m+1}=A_{1}+1$. This is possible because of the form (14) and (15) of coefficients $\alpha_{k}$ and $\beta_{k}$. Indeed, since $\alpha_{k}=-\beta_{d-k-1}$, the terms of the sum which were attached to the $\beta_{k}$ coefficients can be shifted to indices $k=\lfloor d / 2\rfloor, \ldots, d-1$ and now associated to an $\alpha_{k}$. In the odd case, we should in principle impose that the term $k=\lfloor d / 2\rfloor$ disappears, but it happens naturally since $\alpha_{\lfloor d / 2\rfloor}=0$.

As stated in the main text, finding the classical bound of expression (61) reduces to computing the optimal deterministic strategy. Thus, to describe the difference between the outcomes associated to $A_{x}$ and $B_{y}$, we can assign one value $q$ such that $P\left(A_{x}=B_{y}+k\right)=\delta_{k q}$. As $q$ depends on inputs $x$ and $y$ but not all pairs of $A_{x}$ and $B_{y}$ appear in the Bell expression, we thus define $2 m$ variables $q_{i} \in\{0,1 \ldots, d-1\}$ such that:

$$
\begin{align*}
A_{1}-B_{1} & =q_{1}, \\
B_{1}-A_{2} & =q_{2}, \\
A_{2}-B_{2} & =q_{3}, \\
& \vdots \\
A_{m}-B_{m} & =q_{2 m-1},  \tag{62}\\
B_{m}-A_{1} & =q_{2 m}+1 .
\end{align*}
$$

Due to the chained character of these equations, $q_{2 m}$ must obey a superselection rule involving the other $q_{i}$ 's, which is

$$
\begin{equation*}
q_{2 m}=-1-\sum_{i=1}^{2 m-1} q_{i} \tag{63}
\end{equation*}
$$

where the sum is modulo $d$. Due to the fact that the dependence of the coefficients $\alpha_{k}$ on $k$ is only through the cotangent function, proving Theorem 1 boils down to the following maximization problem.

Theorem 1. Let

$$
\hat{\alpha}_{k}:=\cot \left[\frac{\pi}{d}\left(k+\frac{1}{2 m}\right)\right],
$$

and let

$$
\begin{equation*}
\hat{C}_{b}:=\max _{0 \leq q_{1}, \ldots, q_{2 m-1}<d}\left(\sum_{i=1}^{2 m-1} \hat{\alpha}_{q_{i}}+\hat{\alpha}_{-1-\sum_{i=1}^{2 m-1} q_{i}} \bmod d\right) . \tag{64}
\end{equation*}
$$

Then, $\hat{C}_{b}=(2 m-1) \hat{\alpha}_{0}+\hat{\alpha}_{d-1}$.
Notice that to recover the exact expression $\widetilde{C}_{b}$ from the main text, one needs to reintroduce the constant factors appearing in the definition of $\alpha_{k}$ and use Eq. (50). To prove the theorem, we first demonstrate two lemmas. Note that throughout this appendix, we assume that $m \geq 2$ and $d \geq 2$. Although these are not tight conditions to prove our results, they are in any case satisfied by the definition of a Bell test.

Lemma 1. Let $g(x)=\cot \left[\pi\left(x+\frac{1}{2 m}\right) / d\right]$. For all $x$, $y$ satisfying $0 \leq x<y<d-\frac{1}{2 m}$, we have

$$
\begin{equation*}
(1+2 m x) g(x)>(1+2 m y) g(y) \tag{65}
\end{equation*}
$$

Proof. Let us consider the function $f(z):=z \cot z$, which is strictly decreasing in the interval $0<z<\pi$. This can be shown for instance by noting that $f$ is holomorphic and by studying the sign of the coefficients of its Laurent series in a ball of radius $\pi$ centered at $z=0$. Thus, for every $c \in(0, \pi), f(c)>f(z)$ for all $c<z<\pi$. In particular, we can pick $c:=\frac{\pi}{2 d m}(1+2 m x)$ so that:

$$
\begin{equation*}
\frac{\pi}{2 d m}(1+2 m x) \cot \left(\frac{\pi}{2 d m}(1+2 m x)\right)>z f(z) \tag{66}
\end{equation*}
$$

for $\frac{\pi}{2 d m}(1+2 m x)<z<\pi$. By introducing the change of variables $z=\frac{\pi}{2 d m}(1+2 m y)$, equation (65) follows. Note that for integer values of $x$ and $y$, namely $k$ and $l$, Lemma 1 becomes:

$$
\begin{equation*}
(1+2 M k) \hat{\alpha}_{k}>(1+2 M l) \hat{\alpha}_{l}, \quad \forall 0 \leq k<l<d \tag{67}
\end{equation*}
$$

Lemma 2. For integer indices $k, l, p$ such that $0<k, l<d$ and $0 \leq p<d$, we have:

$$
\begin{equation*}
\hat{\alpha}_{0}+\hat{\alpha}_{p}>\hat{\alpha}_{k}+\hat{\alpha}_{l} . \tag{68}
\end{equation*}
$$

Proof. Because all the alphas are ordered $\hat{\alpha}_{0}>\hat{\alpha}_{1}>\hat{\alpha}_{2}>\cdots>\hat{\alpha}_{d-1}$, we have that $\hat{\alpha}_{0}+\hat{\alpha}_{p} \geq$ $\hat{\alpha}_{0}+\hat{\alpha}_{d-1}$ and $\hat{\alpha}_{1}+\hat{\alpha}_{1} \geq \hat{\alpha}_{k}+\hat{\alpha}_{l}$. Hence, it suffices to prove that

$$
\begin{equation*}
\hat{\alpha}_{0}+\hat{\alpha}_{d-1}>2 \hat{\alpha}_{1} \tag{69}
\end{equation*}
$$

Let us rewrite this inequality using the function $g$ introduced in Lemma 1. To this end, we note that the symmetry of the function $\cot (x)=-\cot (-x)$ translates to $g(x)$ in the following manner : $g(x)=-g(-x-1 / m)$. Thus, in order to prove (69), we need to show:

$$
\begin{equation*}
g(0)>2 g(1)+g(1-1 / m) \tag{70}
\end{equation*}
$$

Using Lemma 1 twice, we can express that:

$$
\begin{equation*}
g(0)>(2 m-1) g(1-1 / m)>g(1-1 / m)+2(m-1) \frac{(1+2 m)}{(2 m-1)} g(1) \tag{71}
\end{equation*}
$$

To obtain the second inequality, one of the $2 m-1$ terms was isolated, and Lemma 1 was applied only on the remaining $2(m-1)$ terms. The minimum of $2(m-1)(1+2 m) /(2 m-1)$ is found for $m=2$ and it is equal to $10 / 3$. Since $g(1)$ is positive, and $10 / 3>2$, we can conclude that $g(0)>g(1-1 / m)+2 g(1)$, which is exactly relation (70).

Proof of Theorem 1. To demonstrate the theorem, we employ a dynamical programming procedure which allows us to rewrite Eq. (64) as a chain of maximizations, each over a single variable. Let us first define

$$
\begin{equation*}
h(x):=\max _{0 \leq y<d}\left(\hat{\alpha}_{y}+\hat{\alpha}_{-1-x-y}\right), \tag{72}
\end{equation*}
$$

where the indices are taken to be modulo $d$. As a direct consequence of Lemma $2, h(x)=$ $\hat{\alpha}_{0}+\hat{\alpha}_{-1-x}$. Indeed, the lemma implies that $\hat{\alpha}_{0}+\hat{\alpha}_{-1-x}>\hat{\alpha}_{y}+\hat{\alpha}_{-1-x-y}$ if $y>0$ and
$x \neq d-1-y$. For the cases where $y=0$ or $x=d-1-y$, the maximum is directly attained. This allows us to write the classical bound as:

$$
\begin{equation*}
\hat{C}_{b}=\max _{q_{1}}\left(\hat{\alpha}_{q_{1}}+\max _{q_{2}}\left(\hat{\alpha}_{q_{2}}+\ldots+\max _{q_{2 m-2}}\left(\hat{\alpha}_{q_{2 m-2}}+h\left(\sum_{i=1}^{2 m-2} q_{i}\right)\right) \ldots\right)\right) . \tag{73}
\end{equation*}
$$

Using the properties of $h$, we find that

$$
\begin{equation*}
\max _{q_{k}}\left[\hat{\alpha}_{q_{k}}+h\left(\sum_{i=1}^{k} q_{i}\right)\right]=\hat{\alpha}_{0}+h\left(\sum_{i=1}^{k-1} q_{i}\right) \tag{74}
\end{equation*}
$$

for all $k$. By applying this step $2(m-1)$ times to expression (73), we obtain:

$$
\begin{equation*}
\hat{C}_{b}=(2 m-2) \hat{\alpha}_{0}+h(0)=(2 m-1) \hat{\alpha}_{0}+\hat{\alpha}_{-1} . \tag{75}
\end{equation*}
$$

## D Tsirelson bound of the inequalities

We give here a few more details on the SOS decomposition of any Bell operator corresponding to our new Bell inequality $\widetilde{I}_{d, m}$. Concretely, we show that the identity (18), which we restate here as

$$
\begin{equation*}
\widetilde{Q}_{b} \mathbb{1}-\mathcal{B}=\frac{1}{2} \sum_{i=1}^{m} \sum_{k=1}^{d-1} P_{i k}^{\dagger} P_{i k}+\frac{1}{2} \sum_{i=1}^{m-2} \sum_{k=1}^{d-1} T_{i k}^{\dagger} T_{i k} \tag{76}
\end{equation*}
$$

is valid independently of the choice of $A_{i}^{k}$ and $B_{i}^{k}$. The operators are thus not specified. Here, $P_{i k}=\mathbb{1} \otimes \bar{B}_{i}^{k}-\left(A_{i}^{k}\right)^{\dagger} \otimes \mathbb{1}$, and

$$
\begin{equation*}
T_{i k}=\mu_{i, k} B_{2}^{d-k}+\nu_{i, k} B_{i+2}^{d-k}+\tau_{i, k} B_{i+3}^{d-k} \tag{77}
\end{equation*}
$$

where the coefficients $\mu_{i k}, \nu_{i k}$ and $\tau_{i k}$ are given by

$$
\begin{align*}
\mu_{i, k} & =\frac{\omega^{(i+1)(d-2 k) / 2 m}}{2 \cos (\pi / 2 m)} \frac{\sin (\pi / m)}{\sqrt{\sin (\pi i / m) \sin [\pi(i+1) / m]}} \\
\nu_{i, k} & =-\frac{\omega^{(d-2 k) / 2 m}}{2 \cos (\pi / 2 m)} \sqrt{\frac{\sin [\pi(i+1) / m]}{\sin (\pi i / m)}} \\
\tau_{i, k} & =\frac{1}{2 \cos (\pi / 2 m)} \sqrt{\frac{\sin (\pi i / m)}{\sin [\pi(i+1) / m]}}=-\frac{\omega^{(d-2 k) / 2 m}}{4 \cos ^{2}(\pi / 2 m)} \nu_{i k}^{-1} \tag{78}
\end{align*}
$$

for $i=1, \ldots, m-3$ and $k=1, \ldots, d-1$, while for $i=m-2$ and $k=1, \ldots, d-1$ they are given by

$$
\begin{align*}
\mu_{m-2, k} & =-\frac{\omega^{-(d-2 k) / 2 m}}{2 \sqrt{2} \cos (\pi / 2 m) \sqrt{\cos (\pi / m)}} \\
\nu_{m-2, k} & =-\frac{\omega^{k} \omega^{(d-2 k) / 2 m}}{2 \sqrt{2} \cos (\pi / 2 m) \sqrt{\cos (\pi / m)}} \\
\tau_{m-2, k} & =\frac{\sqrt{\cos (\pi / m)}}{\sqrt{2} \cos (\pi / 2 m)} \tag{79}
\end{align*}
$$

Now, in order to check the validity of the SOS decomposition (76) let us first introduce the explicit form of $P_{i k}$ into the first term of the right-hand side of (76), which gives

$$
\begin{equation*}
\sum_{i=1}^{m} \sum_{k=1}^{d-1} P_{i k}^{\dagger} P_{i k}=\widetilde{Q}_{b} \mathbb{1}-2 \mathcal{B}+\mathbb{1} \otimes \sum_{i=1}^{m} \sum_{k=1}^{d-1}\left(\bar{B}_{i}^{k}\right)^{\dagger}\left(\bar{B}_{i}^{k}\right) \tag{80}
\end{equation*}
$$

where we have used the fact that the Bell operator $\mathcal{B}$ is Hermitian.
Let us then introduce the explicit form of the operators $T_{i k}$ into the last term of the righthand side of (76), which, after some simple algebra, leads us to

$$
\begin{align*}
\sum_{i=1}^{m-2} \sum_{k=1}^{d-1} T_{i k}^{\dagger} T_{i k}= & \sum_{i=1}^{m-2} \sum_{k=1}^{d-1}\left(\left|\mu_{i, k}\right|^{2}+\left|\nu_{i, k}\right|^{2}+\left|\tau_{i, k}\right|^{2}\right) \mathbb{1} \\
& +\sum_{k=1}^{d-1}\left[\mu_{1, k}^{*} \nu_{1, k}\left(B_{2}^{d-k}\right)^{\dagger}\left(B_{3}^{d-k}\right)+\mu_{1, k} \nu_{1, k}^{*}\left(B_{3}^{d-k}\right)^{\dagger}\left(B_{2}^{d-k}\right)\right] \\
& +\sum_{k=1}^{d-1}\left[\mu_{m-2, k}^{*} \tau_{m-2, k}\left(B_{2}^{d-k}\right)^{\dagger}\left(B_{1}^{d-k}\right)+\mu_{m-2, k} \tau_{m-2, k}^{*}\left(B_{1}^{d-k}\right)^{\dagger}\left(B_{2}^{d-k}\right)\right] \\
& +\sum_{i=1}^{m-3} \sum_{k=1}^{d-1}\left[\left(\mu_{i, k}^{*} \tau_{i, k}+\mu_{i+1, k}^{*} \nu_{i+1, k}\right)\left(B_{2}^{d-k}\right)^{\dagger}\left(B_{i+3}^{d-k}\right)\right. \\
& \left.+\left(\mu_{i, k} \tau_{i, k}^{*}+\mu_{i+1, k} \nu_{i+1, k}^{*}\right)\left(B_{i+3}^{d-k}\right)^{\dagger}\left(B_{2}^{d-k}\right)\right] \\
& +\sum_{i=1}^{m-2} \sum_{k=1}^{d-1}\left[\nu_{i, k}^{*} \tau_{i, k}\left(B_{i+2}^{d-k}\right)^{\dagger}\left(B_{i+3}^{d-k}\right)+\nu_{i, k} \tau_{i, k}^{*}\left(B_{i+3}^{d-k}\right)^{\dagger}\left(B_{i+2}^{d-k}\right)\right] \tag{81}
\end{align*}
$$

Now, it follows from Eqs. (78) and (79) that $\mu_{i, k}^{*} \tau_{i, k}+\mu_{i+1, k}^{*} \nu_{i+1, k}=0$ for $i=1, \ldots, m-3$ and $k=$ $1, \ldots, d-1$, which means that the fourth and fifth lines in the above vanish. Then, one notices that $\mu_{1, k}^{*} \nu_{1, k}=\mu_{m-2, k} \tau_{m-2, k}^{*}=\nu_{i, k}^{*} \tau_{i, k}=-a_{k}^{2}$ for $i=1, \ldots, m-3$ and $k=1, \ldots, d-1$, and $\nu_{m-2, k} \tau_{m-2, k}^{*}=-\omega^{k}\left(a_{k}^{*}\right)^{2}$ for $k=1, \ldots, d-1$, where, as before, $a_{k}=\omega^{-(d-2 k) / 4 m} /[2 \cos (\pi / 2 m)]$. Therefore, the remaining terms on the right-hand side of Eq. (81) can be wrapped up as

$$
\begin{align*}
\sum_{i=1}^{m-2} \sum_{k=1}^{d-1} T_{i k}^{\dagger} T_{i k}= & \sum_{i=1}^{m-2} \sum_{k=1}^{d-1}\left(\left|\mu_{i k}\right|^{2}+\left|\nu_{i k}\right|^{2}+\left|\tau_{i k}\right|^{2}\right) \mathbb{1} \\
& -\sum_{i=1}^{m-1} \sum_{k=1}^{d-1}\left[a_{k}^{2}\left(B_{i}^{d-k}\right)^{\dagger}\left(B_{i+1}^{d-k}\right)+\left(a_{k}^{*}\right)^{2}\left(B_{i+1}^{d-k}\right)^{\dagger}\left(B_{i}^{d-k}\right)\right] \\
& -\sum_{k=1}^{d-1}\left[\omega^{k}\left(a_{k}^{*}\right)^{2}\left(B_{1}^{d-k}\right)^{\dagger}\left(B_{m}^{d-k}\right)+\omega^{-k} a_{k}^{2}\left(B_{m}^{d-k}\right)^{\dagger}\left(B_{1}^{d-k}\right)\right] . \tag{82}
\end{align*}
$$

By substituting Eqs. (80) and (82) into Eq. (76) and exploiting the explicit form of the operators $\bar{B}_{i}^{k}$, one obtains

$$
\begin{align*}
\frac{1}{2} \sum_{i=1}^{m} \sum_{k=1}^{d-1} P_{i k}^{\dagger} P_{i k}+\frac{1}{2} \sum_{i=1}^{m-2} \sum_{k=1}^{d-1} T_{i k}^{\dagger} T_{i k}= & \frac{1}{2} \widetilde{Q}_{b} \mathbb{1}-\mathcal{B} \\
& +\sum_{k=1}^{d-1}\left[m\left|a_{k}\right|^{2}+\frac{1}{2} \sum_{i=1}^{m-2}\left(\left|\mu_{i, k}\right|^{2}+\left|\nu_{i, k}\right|^{2}+\left|\tau_{i, k}\right|^{2}\right)\right] \mathbb{1} \tag{83}
\end{align*}
$$

It is easy to finally realize that the last two terms in the above formula amount to $(1 / 2) \widetilde{Q}_{b}=$ $(1 / 2) m(d-1)$, which completes the proof.

## E No-signalling bound of the inequalities

As for the proof of the classical bound we start from the Bell expression written as:

$$
\begin{equation*}
I_{d, m}:=\sum_{k=0}^{d-1} \alpha_{k} \sum_{i=1}^{m}\left[P\left(A_{i}=B_{i}+k\right)+P\left(B_{i}=A_{i+1}+k\right)\right], \tag{84}
\end{equation*}
$$

with $A_{m+1}=A_{1}+1$. Following considerations from Appendix C, the coefficient $\alpha_{0}$ is the biggest of the sum. Clearly, the algebraic bound of $I_{d, m}$ is then $2 m \alpha_{0}$. To complete the proof, we provide a no-signalling behaviour that reaches this bound. Let us recall the no-signalling conditions for a probability distribution:

$$
\begin{align*}
\sum_{b} P\left(A_{x}=a, B_{y}=b\right)=\sum_{b} P\left(A_{x}=a, B_{y^{\prime}}=b\right) & \forall a, x, y, y^{\prime} \\
\sum_{a} P\left(A_{x}=a, B_{y}=b\right)=\sum_{a} P\left(A_{x^{\prime}}=a, B_{y}=b\right) & \forall b, y, x, x^{\prime} \tag{85}
\end{align*}
$$

which express that the marginals on Alice's side do not depend on Bob's input, and conversely. The behaviour that we present is the following. For inputs $x$ and $y$ such that $x=y$ or $x=y+1$ :

$$
P\left(A_{y}=a, B_{y}=b\right)=P\left(A_{y+1}=a, B_{y}=b\right)=\left\{\begin{array}{cll}
1 / d & \text { if } & a=b  \tag{86}\\
0 & \text { if } & a \neq b
\end{array}\right.
$$

There is a special case for $x=1$ and $y=m$ :

$$
P\left(A_{1}=a, B_{m}=b\right)=\left\{\begin{array}{cll}
1 / d & \text { if } & a=b-1  \tag{87}\\
0 & \text { if } & a \neq b-1
\end{array}\right.
$$

where the addition is modulo $d$. For all the other input combinations (i.e. the ones not appearing in the inequalities), we have:

$$
\begin{equation*}
P\left(A_{x}=a, B_{y}=b\right)=1 / d^{2} \quad \forall a, b \tag{88}
\end{equation*}
$$

One can easily verify that this distribution satisfies conditions (85). To obtain the expression from Theorem 3, it suffices to write explicitly $2 m \alpha_{0}$ and to use relation (50).

## F Scaling of the bounds

Here, we study the asymptotic behaviour of the bounds of our Bell expressions for large numbers of inputs $m$ and outputs $d$. We also show that for any values of $m$ and $d$, the classical bound is strictly smaller than the quantum bound, which is strictly smaller than the no-signalling bound. This ensures in particular that the Bell inequality is never trivial.

Let us start with the quantity:

$$
\begin{equation*}
\frac{\widetilde{Q}_{b}}{\widetilde{C}_{b}}=\frac{2 m(d-1)}{\tan \left(\frac{\pi}{2 m}\right)\left[(2 m-1) \cot \left(\frac{\pi}{2 d m}\right)-\cot \left(\frac{\pi}{d}\left(1-\frac{1}{2 m}\right)\right)\right]-m} \tag{89}
\end{equation*}
$$

which is the ratio between the quantum and classical bounds. We also consider the ratio between the no-signalling and quantum bounds, which is:

$$
\begin{equation*}
\frac{\widetilde{N S}_{b}}{\widetilde{Q}_{b}}=\frac{\tan \left(\frac{\pi}{2 m}\right) \cot \left(\frac{\pi}{2 d m}\right)-1}{d-1} \tag{90}
\end{equation*}
$$

To observe the behaviour of these quantities for high number of inputs $m$ and outputs $d$, we can use the Taylor series expansion in two variables, $1 / m$ and $1 / d$, and keep the dominant terms. We obtain:

$$
\begin{align*}
\frac{\widetilde{Q}_{b}}{\widetilde{C}_{b}} & =1+\frac{1}{2 m}-\frac{\pi^{2}-6}{12 m^{2}}+\cdots  \tag{91}\\
\frac{\widetilde{N S}_{b}}{\widetilde{Q}_{b}} & =1+\frac{\pi^{2} / 12-\pi^{2} / 12 d^{2}}{m^{2}}+\cdots \tag{92}
\end{align*}
$$

Thus, when the parameters $m$ and $d$ are of the same order and both very large, i.e. $m=\Theta(d)$, both ratios tend to 1 . It is interesting to consider how fast the bounds tend towards each other: since the ratio between the no-signalling and quantum bounds lacks a term in $1 / m$, it is clear that the quantum bound approaches the no-signalling bound faster than the classical bound approaches the quantum bound.

If we fix the number of outputs $d$ and consider the limit of a large number of inputs $m$, the ratios still tend to 1 . However, if we fix $m$ and considers the limit of large $d$, both ratios tend to constants which are a bit bigger than 1 . They are :

$$
\begin{align*}
\lim _{d \rightarrow \infty} \widetilde{Q}_{b} / \widetilde{C}_{b} & =\frac{(2 m-1) \pi \cot (\pi / 2 m)}{4 m(m-1)}  \tag{93}\\
\lim _{d \rightarrow \infty} \widetilde{N S}_{b} / \widetilde{Q}_{b} & =\frac{2}{\pi} m \tan \left(\frac{\pi}{2 m}\right) \tag{94}
\end{align*}
$$

It is worth mentioning that both functions of $m$ appearing on the right-hand sides of the above formulas attain their maxima for $m=2$ which are $4 / \pi$ and $3 \pi / 8$, respectively. To give the reader more insight, we present in Tables 1 and 2 the numerical values of these ratios for low values of $m$ and $d$.

Now, let us show that these ratios are strictly larger than 1 for any value of $m$ and $d$ consistent with a Bell scenario.

Lemma 3. For any $m, d \geq 2$, the quantum bound of $\widetilde{I}_{d, m}$ is strictly larger than the classical one, that is,

$$
\begin{equation*}
\widetilde{Q}_{b} / \widetilde{C}_{b}>1 \tag{95}
\end{equation*}
$$

Proof. We prove that $\widetilde{Q}_{b}-\widetilde{C}_{b}>0$, which is equivalent to (95) since both bounds are larger than 0 . This inequality can be written as:

$$
\begin{equation*}
2 m d \cot \left(\frac{\pi}{2 m}\right)-2 m \cot \left(\frac{\pi}{2 d m}\right)+\cot \left(\frac{\pi}{2 d m}\right)+\cot \left(\frac{\pi}{d}\left(1-\frac{1}{2 m}\right)\right)>0 \tag{96}
\end{equation*}
$$

If we define $a=1 / d$ and $x=\pi / 2 m$, it becomes:

$$
\begin{equation*}
a x \cot (a(\pi-x))+a(x-\pi) \cot (a x)+\pi \cot (x)>0 \tag{97}
\end{equation*}
$$

for $0<a \leq 1 / 2$ and $0<x \leq \pi / 4$. Since the first term is positive for these intervals, it suffices to show that

$$
\begin{equation*}
u(a, x):=a(x-\pi) \cot (a x)+\pi \cot (x)>0 \tag{98}
\end{equation*}
$$

Clearly, $u(a, x) \geq \min _{a}(u(a, x))$. This minimum corresponds to the limit $a \rightarrow 0$, since the derivative $\partial u(a, x) / \partial a$ of $u(a, x)$ with respect to $a$ is strictly positive on the considered intervals of $a$ and $x$. Indeed, it holds that

$$
\begin{equation*}
\frac{\partial u(a, x)}{\partial a}=(x-\pi) \cot (a x)-\frac{a x(x-\pi)}{\sin ^{2}(a x)} \tag{99}
\end{equation*}
$$

which can be rewritten as

$$
\begin{equation*}
\frac{\partial u(a, x)}{\partial a}=\frac{\pi-x}{2 \sin ^{2}(a x)}[2 a x-\sin (2 a x)] \tag{100}
\end{equation*}
$$

Now, due to the fact that $y>\sin y$ for $0<y \leq \pi / 8$, one has that $2 a x>\sin (2 a x)$ for $0<a \leq 1 / 2$ and $0<x \leq \pi / 4$, and therefore the right-hand side of Eq. (100) is strictly positive within the above intervals.

Now, computing the limit of $u(a, x)$ when $a \rightarrow 0$, one obtains

$$
\begin{equation*}
\lim _{a \rightarrow 0} u(a, x)=1-\frac{\pi}{x}+\pi \cot (x) \tag{101}
\end{equation*}
$$

It can be verified straightforwardly that this expression is strictly positive in the interval $0<$ $x \leq \pi / 4$, by comparing the two functions $\pi \cot (x)$ and $\frac{\pi}{x}-1$, and noticing that the former upper bounds the latter in the interval $0<x \leq \pi / 4$. Indeed, at $x=\pi / 4$, we have that $\pi \cot (\pi / 4)>3$, and in this interval, both their derivatives are negative, with the derivative of the first function smaller than the derivative of the second one. Thus, $u(a, x)>0$.

Lemma 4. For any $m, d \geq 2$, the no-signalling bound of $\tilde{I}_{d, m}$ is strictly larger than the quantum one, that is,

$$
\begin{equation*}
\widetilde{N S} \widetilde{Q}_{b}>1 \tag{102}
\end{equation*}
$$

Proof. Writing the inequality explicitely as in (90), it follows that it is enough to show that $\tan (\pi / 2 m) \cot (\pi / 2 d m)>d$. Let us prove a slightly simpler inequality:

$$
\begin{equation*}
\tan (\pi / 2 m)>d \tan (\pi / 2 d m) \tag{103}
\end{equation*}
$$

To this end, we show that $\tan (a x)>a \tan (x)$ for any $0<x \leq \pi / 2 a$ and any integer $a \geq 2$. We notice that for $x=0, \tan (0)=a \tan (0)$, and that $[\tan (a x)]^{\prime} \geq[a \tan (x)]^{\prime} \geq 0$, meaning that both $\tan (a x)$ and $a \tan (x)$ are monotonically increasing functions and that the former grows faster than the latter. The inequality for the derivatives holds true because $\cos (x)$ is a monotonically decreasing function for $0 \leq x \leq \pi / 2 a$ which implies that $\cos (x) \geq \cos (a x)$.

To complete the proof we note that $\tan (\pi / 2 m)=\tan [d(\pi / 2 d m)]$ and using $x=\pi / 2 d m$ and $a=d$, one can exploit the above inequality to obtain Eq. (103). This finally implies Eq. (102).

|  | m | 2 | 3 | 4 | 5 | 6 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2 | 1.414 | 1.299 | 1.232 | 1.189 | 1.159 |  |
| 3 | 1.291 | 1.214 | 1.167 | 1.137 | 1.116 |  |
| 4 | 1.252 | 1.186 | 1.146 | 1.120 | 1.102 |  |
|  | 5 | 1.233 | 1.173 | 1.136 | 1.112 | 1.095 |
|  |  | 1.222 | 1.165 | 1.130 | 1.107 | 1.091 |

Table 1: Numerical values of the ratio $\widetilde{Q}_{b} / \widetilde{C}_{b}$ for low number of inputs $m$ and outputs $d$. For $m=d=2$, one recovers the well-known CHSH $\sqrt{2}$ ratio.

| 2 | m | 2 | 3 | 4 | 5 | 6 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2 | 1.414 | 1.155 | 1.082 | 1.051 | 1.035 |  |
| 3 | 1.366 | 1.137 | 1.073 | 1.046 | 1.031 |  |
| 4 | 1.342 | 1.128 | 1.069 | 1.043 | 1.029 |  |
|  |  | 1.328 | 1.123 | 1.066 | 1.041 | 1.028 |
|  |  | 1.319 | 1.120 | 1.064 | 1.040 | 1.027 |

Table 2: Numerical values of the ratio $\widetilde{N S}{ }_{b} / \widetilde{C}_{b}$ for low number of inputs $m$ and outputs $d$. For $m=d=2$, one recovers the well-known CHSH $\sqrt{2}$ ratio.

